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HIGH PRODUCTION VOLUME (HPV)

CHEMICAL INITIATIVE

Analysis Document and Testing Plan

For

ARYLPOLYOLEFINS

Prepared by
The American Chemistry Council
Petroleum Additives Panel
Health, Environmental, and Regulatory Task Group

November 26, 2002

LIST OF MEMBER COMPANIES IN THE HEALTH, ENVIRONMENTAL AND REGULATORY TASK GROUP

The Health, Environmental, and Regulatory Task Group (HERTG) of the American Chemistry Council Petroleum Additives Panel includes the following member companies:

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The Lubrizol Corporation

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EXECUTIVE SUMMARY

The American Chemistry Council Petroleum Additives Panel Health, Environmental, and Regulatory Task Group (HERTG), and its member companies, hereby submit for review this category analysis document and testing plan for the *"arylpolyolefins"* under the International Council of Chemical Associations (ICCA) Initiative on High Production Volume (HPV) chemicals. This report should be read in its entirety in order to obtain a complete understanding of the category and proposed testing.

Arylpolyolefins. Relying on several factors specified in the OECD guidance document on "Development of Chemical Categories in the HPV Challenge Program," in which use of chemical categories is encouraged, the following two closely related high production volume chemicals are submitted as a category:

- Benzene, C_{14}-C_{24}-branched and linear alkyl derivatives (CAS # 115733-08-9) referred to in this report as the "C_{14}-C_{24} alkaryl derivative."
- Benzene, polypropene derivatives (CAS # 68081-77-6) referred to in this report as the "polypropene derivative."

Structural Similarity. A key factor that supports these chemicals as a category is their structural similarity. The two category members are composed of chemical constituents that contain one aromatic ring to which an alkyl group is attached. The alkyl group is either linear or methyl branched and ranges in carbon (C) number from C_{14} to approximately C_{82}.

Similarity of Physicochemical Properties. The physicochemical properties of these substances are generally similar or overlap and can be explained by their similarities in chemical structure and chemical processing. They are clear to yellow-colored liquids at ambient temperatures and have high boiling points. These substances have low volatility due to their low vapor pressure and relatively high molecular weights. Arylpolyolefins have low water solubility and have high Kow values.

Fate and Transport Characteristics. The potential of the members of the arylpolyolefin category to biodegrade varies in accordance with their chemical structure. Category members with linear alkyl side chains are expected to biodegrade to a high extent, but category members with branched alkyl side chains are expected to have a limited potential to biodegrade. Since members of this category have low water solubility, hydrolysis testing is technically unfeasible. Furthermore, category members are resistant to hydrolysis because they lack hydrolyzable moieties. Component molecules of category members do not absorb sufficient light energy to result in a structural transformation, therefore they are not subject to direct photolytic reactions. Although arylpolyolefins have a low potential to partition to the air to a significant degree because of their low vapor pressure, computer-modeled data characterizing the atmospheric oxidation potential (indirect photodegradation) for category members suggest that they will degrade rapidly in air. These substances are not expected to partition to water or air if released into the environment due to their low water solubility and low vapor pressure, and partitioning data suggest that chemical components of category members will partition primarily to soil.

Toxicological Similarity. Review of existing published and unpublished test data for members of this category shows predominantly low mammalian toxicity as discussed below.

> *Aquatic Toxicology.* Aquatic toxicity data are not available to characterize category members. Therefore, data will be developed to characterize the fish, invertebrate and alga toxicity of category members.
>
> *Mammalian Toxicology - Acute.* Data on acute mammalian toxicity were reviewed. The findings indicate a low degree of acute toxicity. Data are available for both members of the arylpolyolefin category indicating that the category has been well tested for acute mammalian effects. Therefore, no additional acute mammalian toxicity testing is necessary.
>
> *Mammalian Toxicology - Genotoxicity.* An *in vitro* bacterial gene mutation assay was reviewed for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9). The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) did not demonstrate mutagenic activity in either the presence or absence of metabolic activation. This test will be used for bridging to the other category member. No chromosomal aberration assays are available for the members of the arylpolyolefin category. It is recommended that an *in vitro* chromosomal aberration assay be conducted for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the results bridged to the other category member.
>
> *Mammalian Toxicology - Subchronic Toxicity.* There are no repeated-dose toxicity studies available for the members of the arylpolyolefin category. It is recommended that an oral repeated-dose toxicity study be conducted for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the results bridged to the other category member.
>
> *Mammalian Toxicology - Reproductive and Developmental Toxicity.* There are no reproductive or developmental toxicity studies available for the members of the arylpolyolefin category. It is recommended that a reproductive/developmental toxicity study be conducted for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the results bridged to the other category member.

Conclusion. Based upon the data reviewed for this category analysis document, it is concluded that the existing physicochemical and toxicological properties of the arylpolyolefins are similar or overlap as a result of their structural relatedness. Thus, these chemicals are considered to constitute a category and additional data will be developed in accordance with the arylpolyolefin test plan summarized below.

Testing Plan. The test plan for the arylpolyolefin category includes the following:

- Water solubility – Solubility data will be developed for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and will be used to characterize the water solubility of the other category member. The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) is the lower molecular weight category member and likely to have the highest water solubility.

- Biodegradation - Biodegradation data will be developed for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and will be used to characterize the biodegradability of the other category member. The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) is the lower molecular weight, more water-soluble category member and has the potential to exhibit the greatest extent of biodegradability.
- Aquatic Toxicity – Acute toxicity testing with a freshwater fish, invertebrate and alga will be conducted on the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and will be used to characterize the aquatic toxicity of the other category member.
- Mutagenicity – An *in vitro* chromosomal aberration study will be conducted on the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the results will be bridged to the other category member.
- Systemic toxicity – An oral repeated-dose toxicity study will be conducted on the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the results will be bridged to the other category member.
- Reproductive/developmental toxicity – A reproductive/developmental toxicity study will be conducted on the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the results will be bridged to the other category member.

As this test plan was developed, careful consideration was given to the number of animals that would be required for tests included in the proposed plan and conditions to which the animals might be exposed. In consideration of the concerns of some non-governmental organizations about animal welfare, the use of animals in this proposed test plan has been minimized.

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1.0 INTRODUCTION

In March 1999, the American Chemistry Council (formerly the Chemical Manufacturers Association) Petroleum Additives Panel - Health, Environmental, and Regulatory Task Group (HERTG) and its participating member companies committed to address for certain chemicals listed under the United States Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program and the International Council of Chemical Associations (ICCA) Initiative on HPV chemicals. This category analysis document and testing plan follows up on that commitment.

Specifically, this category analysis document and testing plan sets forth how the HERTG intends to address relevant physicochemical, environmental, aquatic and health effects information for the following substances:

- Benzene, C_{14}-C_{24}-branched and linear alkyl derivatives (CAS # 115733-08-9) referred to in this report as the "C_{14}-C_{24} alkaryl derivative."
- Benzene, polypropene derivatives (CAS # 68081-77-6) referred to in this report as the "polypropene derivative."

An analysis of the available data on these chemicals supports the designation of the arylpolyolefins as a "chemical category" as provided in the OECD guidance document entitled, "Development of Chemical Categories in the HPV Challenge Program". This category analysis document provides the basis for that determination, indicates the findings of the data review process, and sets forth a proposed test plan to satisfy parts of the required test battery for endpoints without data that would be considered adequate under the Initiative.

The United States EPA guidance on the HPV Program indicates that the primary purpose of the program is to encourage "the chemical industry . . . to voluntarily compile a Screening Information Data Set (SIDS) on all chemicals on the HPV list" (EPA, "Development of Chemical Categories in the HPV Challenge Program," p. 1). The ICCA HPV Chemical Initiative has the same primary purpose for all chemicals on the ICCA HPV lists. At the same time, both the ICCA and EPA recognize that the "large number of chemicals to be tested makes it important to reduce the number of tests to be conducted, *where this is scientifically justifiable.*" (*Id.*, p. 1) [emphasis added] The next part of the EPA guidance explains where this would be scientifically justifiable:

> One approach is to test closely related chemicals as a group, or category, rather than test them as individual chemicals. In the category approach, *not every chemical needs to be tested for every SIDS endpoint.* However, *the test data finally compiled* for the category must prove adequate to support a screening level hazard-assessment of the category and its members. That is, the *final data set* must allow one to estimate the hazard for the untested endpoints, *ideally* by interpolation between and among the category members. In certain cases, where toxicity is low and no upward trend is expected, extrapolation to the higher category members may be acceptable. (*Id.*, p. 1) [emphasis added].

EPA guidance goes on to state, "The use of categories is encouraged in the Challenge Program and will have a number of benefits." (*Id.*, p. 1) Among the benefits identified in the guidance for the use of categories are "a reduction in testing will result in fewer animals used to test a category of chemicals as opposed to doing each test on each individual chemical," and "there will be . . . economic savings since less testing may be needed for chemicals considered as a category." (*Id.*, p. 1) That guidance also states that categories "accomplish the goal of the Challenge Program – to obtain screening level hazard information – through the strategic application of testing to the category." (*Id*, p. 2)

A similarly stated intent "to reduce the number of tests to be conducted, *where this is scientifically justifiable*" was articulated by the EPA in its draft guidance document titled, "The Use of Structure Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program." [emphasis added].

The EPA "Chemical Categories" guidance defines a "chemical category" as a group of chemicals whose physicochemical and toxicological properties *are likely to* be similar *or* follow a regular pattern as a result of structural similarity." (*Op. Cit.*, p. 2) [emphasis added].

According to the guidance, what is important is that the "structural similarities [among members of the group] *may* create a predictable pattern *in any* or all of the following parameters: physicochemical properties, environmental fate, aquatic effects, and human health effects." (Id., p. 2) [emphasis added]. Thus, it is not necessary for the chemicals in a category to be similar in all respects. Nor must there be conclusive proof that the chemicals in the postulated category will behave identically across all relevant parameters. All that is required for an acceptable category is that there be a *likelihood* of similarity of physicochemical and toxicological properties or a *likelihood* that the chemicals will in some pertinent respect follow a regular pattern as a result of their structural similarity.

In identifying the arylpolyolefin category, the six-step process set out in the EPA guidance on category development was followed. As the information below indicates, the arylpolyolefin category of chemicals clearly satisfies the standards established in that guidance for use of a chemical category:

Step 1: group structurally similar chemicals into a putative category

Step 2: gather relevant published and unpublished literature for each member of the category

Step 3: evaluate the compiled data for adequacy in accordance with the EPA guidance documentation

Step 4: construct matrices of SIDS endpoints versus category members arranged so as to indicate the structural progression of the category (in this case, by increasing molecular weight)

Step 5: evaluate the data to determine whether there is a correlation between category members for each SIDS endpoint

Step 6: make available, to the ICCA and the public, this test plan including the foregoing category rationale and the following data assessment with the proposed testing scheme for the arylpolyolefins.

2.0 CHEMISTRY OF ARYLPOLYOLEFINS

2.1 DESCRIPTION

Arylpolyolefins consist of a benzene ring with one long-chain alkyl substituent group. The alkyl group is a saturated hydrocarbon chain that can vary in length and extent of branching. The chemical names and CAS numbers for the members of the category are presented in Table 1 and the chemical structures are presented in Table 2.

Commercial arylpolyolefins are manufactured by reacting anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. Linear alkylbenzenes use linear alpha olefins with $AlCl_3$ and HF as the preferred catalyst. Branched alkylbenzenes start with a tetrapropenyl (C_3) stream using HF as the preferred catalyst, but triethyl aluminum ($AlEt_3$) has also been used as a catalyst.

2.2 PHYSICOCHEMICAL PROPERTIES

Selected physicochemical properties of arylpolyolefin category members are presented in Table 3. The physicochemical properties of these two substances are generally similar or overlap, as would be expected based upon the similarity in their chemical structure and chemical processing, and thus support consideration of these substances as a category.

2.2.1 Molecular Weight and Alkyl Side Chain Length

The category members range in molecular weight from 275 to 415 daltons for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and 387 to 1228 daltons for the polypropene derivative (CAS # 68081-77-6) (Table 3). The structural variable that is responsible for the range in molecular weight of the category members is the number of carbon atoms in the alkyl chain on the benzene ring.

2.2.2 Specific Gravity

The specific gravity of category members are 0.85 for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and 0.87 for the polypropene derivative (CAS # 68081-77-6) (Table 3).

2.2.3 Viscosity

The viscosity of category members are 21 cSt @ 40°C for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and 93 cSt @ 40°C for the polypropene derivative (CAS # 68081-77-6) (Table 3).

2.2.4 Melting Point

The category members are viscous liquids at ambient temperatures.

2.2.5 Boiling Point

Modeling data[1] indicate that the boiling range of category members can range from 342 to 458°C for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and can be >388°C for the polypropene derivative (CAS # 68081-77-6) (Table 3).

The modeling data for physicochemical endpoints in Sections 2.2.5 to 2.2.7 are presented as ranges for category members, where possible, and are based on the highest and lowest molecular weight derivative in each member. For example, structures representing the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) include a benzene C_{14} alkyl derivative and a benzene C_{24} alkyl derivative. Whereas, structures representing the polypropene derivative (CAS # 68081-77-6) include only the benzene C_{22} polypropene lowest molecular weight derivative; the benzene C_{82} polypropene highest molecular weight derivative has not been modeled as the molecular weight of this derivative falls outside of the applicable range of the EPIWIN modeling program. The idealized structures are shown in Table 2. The physicochemical information used in the modeling is found in Table 3.

2.2.6 Vapor Pressure

Modeling data indicate that the vapor pressure range of category members can range from $1.3e^{-2}$ to $1.7e^{-6}$ Pa at 25 °C for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and can be <$6.2e^{-4}$ Pa at 25 °C for the polypropene derivative (CAS # 68081-77-6) (Table 3).

2.2.7 Water Solubility and Octanol-Water Partition Coefficients

Modeling data indicate that the water solubility range of category members can range from $2.0e^{-4}$ to $4.4e^{-9}$ mg/L at 25 °C for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and can be <$1.2e^{-7}$ mg/L at 25 °C for the polypropene derivative (CAS # 68081-77-6). The low water solubility is consistent with the high lipophilic nature and high molecular weight of these substances. Modeling data indicate that the log of the octanol-water partition coefficients (log K_{ow}) for category members are estimated to be >8.9.

The water solubility of category members will be characterized by conducting a water solubility test with the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9). The data developed for this substance will be used to estimate the water solubility of the polypropene derivative (CAS # 68081-77-6).

3.0 USES OF ARYLPOLYOLEFINS

Arylpolyolefins have a wide range of uses, but they are often employed as non-isolated intermediates for conversion to alkaryl sulfonates (HERTG-HPV Group 3). Other uses of arylpolyolefins include use as base fluids in engine oils, transmission fluids, gear oils, hydraulic fluids and other lubricant fluid applications that require fluidity at low temperatures. Some arylpolyolefins are also used as refrigerant lubricants and thermal transfer fluids.

4.0 EVALUATION OF AVAILABLE PUBLIC AND COMPANY DATA

4.1 Environmental Fate Data

4.1.1 Physicochemical Properties Relevant to Environmental Fate

In order to evaluate the environmental fate of a substance, it is important to understand its potential degradability and partitioning behavior among environmental compartments (i.e., air, soil, sediment, suspended sediment, water and biota).

The physicochemical properties and molecular structure of a chemical will influence the degradation processes it may be subjected to in the environment. Potentially important environmental degradation pathways include biodegradation, hydrolysis and photodegradation. Biodegradation of an organic chemical by bacteria can provide energy and carbon for microbial growth. This process results in a structural change of the chemical. Biodegradation can result in the complete loss of an organic chemical, producing carbon dioxide, mineral salts and water. Hydrolysis is a reaction in which a water molecule or hydroxide ion substitutes for another atom or group of atoms present in an organic chemical resulting in a structural change of that chemical. Chemical photodegradation results in a structural change of a molecule from the absorption of solar radiation.

The physicochemical properties of a substance will also influence the way in which it partitions among environmental compartments (i.e., air, water, soil and sediment). Generally, substances characterized by a low vapor pressure do not partition into air to a great extent. Similarly, substances characterized by a low water solubility do not partition extensively into water. Substances that do not partition into air and water to any great extent tend to partition into soil and sediments.

4.1.2 Biodegradability

4.1.2.1 Testing Methodologies

The potential biodegradability of a substance in water, under aerobic conditions can be assessed using one of the OECD 301 testing guidelines. Chemical biodegradation involves a series of microbial-mediated reactions that can require many different microorganisms acting together to degrade a parent substance. There are several standard test methods that measure primary degradation (i.e., loss of parent chemical) or ultimate degradation (i.e., complete utilization of a substance to produce carbon dioxide, water, mineral salts and microbial biomass). Primary degradation can be determined analytically by measuring dissolved organic carbon (DOC) for water-soluble chemicals, infrared absorbance, or by a chemical-specific detection method. Ultimate degradation (also called mineralization), as mediated by microorganisms, can be determined by measuring oxygen consumption or carbon dioxide evolution relative to the theoretical levels that can be derived based on an elemental analysis of the chemical under investigation.

4.1.2.2 Summary of Available Data

Biodegradation data are not available for members of the arylpolyolefin category. The first category member, the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9), is expected to exhibit a higher extent of biodegradability in comparison to the second category member, the polypropene derivative (CAS # 68081-77-6). A lower extent of biodegradability is expected for the polypropene derivative (CAS # 68081-77-6) because of its higher molecular weight and subsequently lower anticipated water solubility. Low water solubility will limit availability to the degrading microorganisms and therefore will limit the potential extent of degradation possible within the guidelines and 28-day duration of a standard test procedure. Additionally, the degree of methyl branching along the alkyl group of the polypropene derivative (CAS # 68081-77-6) (Table 2) will also contribute to a reduced extent of degradation possible under a standard test procedure.

4.1.2.3 Data Assessment and Test Plan for Biodegradability

Biodegradation testing is proposed for the first category member, the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9). The data developed for this substance will be used to estimate the biodegradability of the polypropene derivative (CAS # 68081-77-6).

4.1.3 Hydrolysis

4.1.3.1 Testing Methodologies

The potential for a substance to hydrolyze in water can be assessed as a function of pH (OECD Guideline 111, Hydrolysis as a Function of pH[1]). When an organic molecule undergoes hydrolysis, a nucleophile (water or hydroxide ion) attacks an electrophile and displaces a leaving group (e.g., halogen, phenoxide). Potentially hydrolyzable groups include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters and sulfonic acid esters[2]. The lack of a suitable leaving group renders compounds resistant to hydrolysis.

4.1.3.2 Summary of Available Data

Published or unpublished hydrolysis studies for members of the arylpolyolefin category are not available. Arylpolyolefins do not contain functional groups that are subject to hydrolytic reactions. Thus, these substances have little, if any, potential for hydrolysis and they are expected to be stable in water.

4.1.3.3 Data Assessment and Test Plan for Hydrolysis

Arylpolyolefins do not contain functional groups that are susceptible to hydrolytic degradative mechanisms. Therefore, testing these substances for hydrolysis is not needed to adequately evaluate this endpoint. A technical discussion for hydrolysis is presented as a robust summary.

4.1.4 Photodegradation

4.1.4.1 Testing and Modeling Methodologies

Photodegradation can occur as a result of direct and indirect mechanisms. Direct photodegradation can be measured in solution using the OECD test guideline 113. Indirect photodegradation can be estimated using a model accepted by the US EPA; this estimation method applies a calculation procedure to determine an atmospheric oxidation potential (AOP) value.

Direct photochemical degradation occurs through the absorbance of solar radiation by a chemical substance. If the absorbed energy is high enough, then the resultant excited state of the chemical may lead to its transformation. A prerequisite for direct photodegradation is the ability of one or more bonds within

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[1] Organization for Economic Cooperation and Development (OECD) (1993) OECD Guidelines for Testing of Chemicals. OECD. Paris, France.
[2] W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt. (1982) Handbook of Chemical Property Estimation Methods. McGraw-Hill Book Co. New York, NY, USA.

a chemical to absorb ultraviolet (UV)/visible light in the 290 to 750 nm range. Light wavelengths longer than 750 nm do not contain sufficient energy to break chemical bonds, and wavelengths below 290 nm are shielded from the earth by the stratospheric ozone layer. Indirect photodegradation also requires light energy as well as a series of chemical reactions that include the reaction of a molecule with hydroxyl radicals (OH-).

For estimation of indirect photodegradation, the computer program AOPWIN (atmospheric oxidation program for Microsoft Windows[3]) is used by the US EPA OPPTS (Office of Pollution Prevention and Toxic Substances). This program calculates a chemical half-life based on an overall OH- reaction rate constant, a 12-hour day and a specific OH- concentration.

4.1.4.2 Summary of Available Data

Published or unpublished direct photodegradation studies for the arylpolyolefin category members are not available. Review of the structures of arylpolyolefins indicates that they do not contain bonds that have a significant potential to absorb UV light above 290 nm. Therefore, the arylpolyolefins are not anticipated to undergo direct photodegradation.

Indirect photodegradation data (calculated AOP values) are available to characterize this endpoint for the arylpolyolefin category members (Table 4). Those data show that the parent chemical components of category members have a relatively short half-life in air, approximately 3 to 6 hours. However, given the low vapor pressure of these products, it is unlikely that this degradation process will contribute to their loss from the environment because the chemical components of these products will not tend to significantly partition to the air where this degradation process occurs. These data suggest that those chemical components that do partition to the air phase will degrade rapidly due to hydroxyl radical attack.

AOP values are presented as ranges for category members, where possible, and are based on the highest and lowest molecular weight derivative in each member. For example, structures representing the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) include a benzene C_{14} alkyl derivative and a benzene C_{24} alkyl derivative. Whereas, structures representing the polypropene derivative (CAS # 68081-77-6) include only the benzene C_{22} polypropene lowest molecular weight derivative; the benzene C_{82} polypropene highest molecular weight derivative has not been modeled as the molecular weight of this derivative falls outside of the applicable range of the EPIWIN modeling program.

[3] EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

4.1.4.3 Data Assessment and Test Plan for Photodegradation

Based on their structures, arylpolyolefins are not anticipated to undergo direct photodegradation. Therefore, no additional testing for direct photodegradation is planned. A technical discussion for this endpoint is presented as a robust summary. For indirect photodegradation, calculated AOP values of selected chemical structures representative of the arylpolyolefin category members are available to characterize this endpoint. Therefore, no additional modeling is planned. The data suggest that the arylpolyolefin category members would be subject to rapid degradation in air from OH- attack. This effect would be limited by the low vapor pressure of these materials.

4.1.5 Fugacity Modeling

4.1.5.1 Modeling Methodologies

Fugacity-based multimedia fate modeling calculates the relative distribution of a chemical between environmental compartments. A widely used model for this approach is the EQC model[4].

There are multiple levels of the EQC model, which vary in complexity and data requirements. In the document, "Determining the Adequacy of Existing Data", EPA states that it accepts Level I fugacity modeling to estimate transport/distribution values. The EQC Level I model utilizes input of basic chemical properties, including molecular weight, vapor pressure and water solubility to calculate the percent distribution of a chemical within a standardized environment (unit world). Another EQC model, the Level III, uses these parameters, as well as chemical emission rates into air, water and soil and chemical degradation rates in air, water, soil and sediment.

4.1.5.2 Summary of Available Data

Published or unpublished fugacity data for the arylpolyolefin category members are not available. Arylpolyolefins have low vapor pressure and low water solubility, which suggests that they will not partition into the air or water to a great extent. Fugacity-based multimedia fate data for the arylpolyolefin category members suggest that these substances will partition to soil (Table 5).

Distribution values are presented as ranges for category members, where possible, and are based on the highest and lowest molecular weight derivative in each member. For example, structures representing the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) include a benzene C_{14} alkyl derivative and a benzene C_{24} alkyl

[4] Mackay, D., A. Di Guardo, S. Paterson, and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15:1627-1637.

derivative. Whereas, structures representing the polypropene derivative (CAS # 68081-77-6) include only the benzene C_{22} polypropene lowest molecular weight derivative; the benzene C_{82} polypropene highest molecular weight derivative has not been modeled as the molecular weight of this derivative falls outside of the applicable range of the EPIWIN modeling program used to generate the physicochemical input data for the EQC Level I fugacity model.

4.1.5.3 Data Assessment and Test Plan for Fugacity

The relative distribution of substances within this category among environmental compartments was evaluated using the EQC Level I model (Table 5). Data developed using an EQC Level I model can be used for simple comparative purposes across several substances. The data suggest that category members will partition primarily to soil.

The EQC Level III model was not used for this evaluation because appropriate emission levels as yet are unknown. Because of the physical nature of the substances in this category, a Level I dataset was adequate to assess the potential partitioning behavior of arylpolyolefin category members in the environment.

Input data to run the EQC Level I model required an additional computer model to estimate selected physicochemical properties from a structure. The model used for this purpose was EPIWIN, version 3.04[5]. EPIWIN includes algorithms for estimating all physical and chemical properties needed for the EQC model.

4.2. ECOTOXICOLOGY DATA

4.2.1 Aquatic Ecotoxicity Testing

4.2.1.1 Test Methodologies

Acute aquatic ecotoxicity testing can include three species that represent three trophic levels in the freshwater aquatic environment: fish, invertebrates and algae. The fish acute toxicity test (OECD Guideline 203, *Fish, Acute Toxicity Test*) determines the lethality of a substance to a fish during a 96-hour exposure period. The invertebrate toxicity test (OECD Guideline 202, *Daphnia sp., Acute Immobilization Test and Reproduction Test*) determines the potential of a substance to immobilize an invertebrate, typically a daphnid (*Daphnia magna*), during a 48-hour exposure period. The alga growth inhibition test (OECD Guideline 201, *Alga, Growth Inhibition Test*) determines the potential of a substance to inhibit alga growth, typically using the freshwater unicellular green

[5] EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

algae, *Pseudokirchneriella subcapitata* (formerly called *Selenastrum capricornutum*), during a 72-or 96-hour exposure period.

Three different exposure methodologies are available to conduct aquatic toxicity tests; i.e., flow-through, static and static renewal.

In *flow-through exposures*, organisms are exposed to a constant chemical concentration or loading in each treatment level in the incoming water and there is typically greater assurance than with other test methods that the exposure levels and water quality remains constant throughout the test. Although flow-through testing is a preferred method, it is most applicable for chemicals that have adequate water solubility.

In *static exposures*, organisms are exposed to a chemical in a test medium that is not replaced for the duration of the study. There is less assurance that the test material concentrations to which test organisms are exposed will remain constant because test material will have a greater opportunity to be lost from the aqueous phase by being adsorbed onto test chambers, degraded, volatilized, or otherwise changed during the test. Nevertheless, due to limitations of other test systems for non-volatile materials, the static test has been widely used and in some instances must be used, as is the case when conducting an alga test.

The *static-renewal exposure* is similar to a static exposure because it is conducted in still water, but the test solutions and control water are renewed periodically, usually every 24 hours. Daily test solution renewal provides a greater likelihood that the exposure concentrations or loadings will remain stable throughout the test. This is the preferred method for conducting fish toxicity tests for compounds such as the arylpolyolefins. Daily renewals cannot be done in the alga test, and dependent on the substance and test procedure used, renewals may not be possible for the *Daphnia* test because the process of exposure solution separation and replenishment can cause a discontinuity in the alga growth rate and it can stress *Daphnia* or result in coating or entrapping the organisms in surface film that may form during renewal operations, respectively. OECD considers the use of static testing for fish, *Daphnia* and algae and the use of static renewal testing for fish to be appropriate when evaluating the toxicity of complex, poorly water-soluble chemicals like arylpolyolefins, provided that test solution preparation uses water accommodated fraction or water soluble fraction preparation methods[6].

4.2.1.2 Test Solution Preparation

Arylpolyolefins are complex, poorly water-soluble substances, and it is not possible to prepare exposure solutions for aquatic toxicity testing by direct

[6] Organization for Economic Cooperation and Development (OECD) (2000). Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures. OECD Environmental Health and Safety Publications, Series on Testing and Assessment No.23, Paris, France.

addition of measured quantities of test material to aqueous media. Two methods are used to prepare solutions of complex, poorly water-soluble materials for aquatic toxicity testing as recommended in the OECD guidance document on testing difficult substances[7]:

- *Water accommodated fraction* (WAF) – This is a method in which the test solution contains only that fraction of the test material (organic phase), which is retained in the aqueous phase after a period of stirring sufficient to reach equilibrium, followed by a sufficient time for phase separation. The WAF (aqueous phase) will contain soluble components of the test material at levels that will be dependent on the test material loading (the amount of material added to the aqueous medium). The resulting WAF is used in the aquatic toxicity test. Ideally, a WAF consists of a water-soluble extract of test material, but it can also include a stable micro-emulsion or contain small amounts of suspended matter.

- *Water soluble fraction* (WSF) – This is a method in which a WAF is either filtered, centrifuged, or allowed to settle for a greater length of time (24 hours) than with the WAF method, to remove suspended matter or emulsions from the aqueous phase before being used in the aquatic toxicity test.

4.2.1.3 Reporting Toxicity Results

In both WAF and WSF tests, test material exposures are expressed as loading rates (i.e., defined as the weight of test material added per unit volume of test medium during WAF or WSF preparation)[7]. For fish tests, endpoints can be expressed as median lethal loading rate (LL_{50}) when lethal effects occur to 50% of the test population. In cases where no lethal effects are observed at all loadings tested, the result may be expressed as: LL_0 = the highest loading tested. In both cases, results can be expressed in mg/L. For invertebrate and alga tests, endpoints are expressed as median effective loading rate (EL_{50}) or EL_0 in mg/L as discussed above.

Loading rates allow complex, poorly water-soluble substances such as the arylpolyolefins to be compared to more readily soluble substances and pure chemicals on an equal basis. To allow comparison, the toxicity value is expressed as the amount of test material added per unit volume of water when preparing the WAF or WSF.

If test material exposure levels are analytically measured in the test, the endpoints can also be expressed as median lethal concentration (LC_{50}) or median effective

[7] Organization for Economic Cooperation and Development (OECD) (2000). Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures. OECD Environmental Health and Safety Publications, Series on Testing and Assessment No.23, Paris, France.

concentration (EC_{50}) in mg/L. When working with complex, poorly water-soluble substances, LC/EC_{50} values are often not determined because it can be very difficult to accurately measure test substance exposure levels below 1.0 mg/L.

4.2.2 Aquatic Toxicity of the Arylpolyolefin Category

In general, the toxicity of a substance to an organism is limited by mechanisms of uptake and movement to target organs. Characteristics such as relative smaller molecular weight and a lesser degree of ionization increase the ability of a substance to passively cross biological membranes and exert effects. However, the water-soluble fraction of a compound represents the fraction to which aquatic organisms in the water column will be exposed and the fraction that is available to cause toxicity. Therefore, aquatic toxicity can be either limited by the water solubility of a substance or not determinable, if that substance has very low solubility.

Modeling data suggest that arylpolyolefins have low water solubility. The low water solubility suggests that the aquatic toxicity of these substances will be limited due to low bioavailability to aquatic organisms. As discussed in Section 2.2.7, water solubility testing will be conducted with one of the arylpolyolefin category substances to ensure that the water solubility of the category has been adequately assessed. Aquatic toxicity testing will be conducted on the substance as marketed.

4.2.2.1 Summary of Available Data

There are no aquatic toxicity data available for the members of the arylpolyolefin category.

4.2.2.2 Data Assessment and Test Plan for Acute Aquatic Ecotoxicity

The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) will be evaluated for acute toxicity to a freshwater fish, invertebrate and alga. The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) will be tested because of its lower molecular weight and subsequently higher anticipated water solubility. The data developed for this substance will be used to estimate the aquatic toxicity of the polypropene derivative (CAS # 68081-77-6).

4.3 MAMMALIAN TOXICOLOGY DATA

4.3.1 Physicochemical Properties Relevant to Mammalian Toxicity

Physicochemical properties of chemicals are useful for predicting the routes by which exposure may occur, and in some cases, the mechanism and extent of toxicological responses. The physicochemical properties of the arylpolyolefins are presented in Table

3. These substances are relatively high molecular weight liquids with high octanol/water partition coefficients, low water solubilities and low vapor pressure.

There is little structural diversity in the arylpolyolefin category (Table 2). The arylpolyolefins are characterized by both polypropenyl (branched alkyl side chains) and linear alkyl side chain species. For health-related endpoints, the length or extent of branching of the alkyl side chain is not expected to influence the index of toxicity.

4.3.2 Acute Mammalian Toxicity of the Arylpolyolefin Category

4.3.2.1 Acute Toxicity Test Methodology

Acute toxicity studies investigate the effect(s) of a single exposure to a relatively high dose of a substance. Potential routes of exposure for acute toxicity assays include oral, dermal and inhalation. Oral toxicity assays are conducted by administering test material to fasted animals (typically rats or mice) as a single gavage dose. Acute dermal toxicity tests are conducted by administering test material to the shaved skin on the back of the test animal (typically rats or rabbits) and allowing the test material to stay in contact with the skin application site for a specific duration (usually 24 hours). Acute inhalation toxicity assays are conducted by exposing test animals (typically rats) in a controlled atmosphere to a fixed air concentration of the test substance for a specific duration (typically 4 hours). The test material is generated as a vapor or intentionally aerosolized into respirable particles, then metered into the exposure air at the desired concentration. Preferably, inhalation toxicity studies are conducted using either nose-only or head-only exposure to minimize potential confounding effects resulting from whole-body exposure. Whole body exposure may lead to over-prediction of inhalation toxicity hazard by increasing the body-burden of the test material through skin absorption or ingestion of test material as a consequence of grooming both during and after the inhalation exposure period.

Historically, lethality is a primary end-point of concern in acute toxicity studies, and the traditional index of oral and dermal potency is the median lethal dose that causes mortality in 50 percent of the test animals (LD_{50}). In acute inhalation studies, the traditional measurement of potency is the median lethal concentration of the test material in air that causes mortality in 50 percent of the test animals (LC_{50}). In addition to lethality, acute toxicity studies also provide insights regarding potential systemic toxicity through careful observation and recording of clinical signs and symptoms of toxicity as well as through detailed examination of tissues and organ systems.

Typically, acute oral and dermal toxicity studies are conducted using a limit dose of 5 and 2 g/kg body weight, respectively, and acute inhalation toxicity studies are conducted using a limit dose of 5 mg/L for 4 hours (according to OECD and EPA testing guidelines). Prior to 1990, some acute dermal toxicity studies may have used a limit dose of 5 g/kg. Recently, harmonized EPA testing guidelines (August

1998) have set the limit dose for both oral and dermal acute toxicity studies at 2 g/kg body weight, while the recommended limit concentration for acute inhalation studies has been set at 2 mg/L for 4 hours. The limit dose test method minimizes the number of animals tested by exposing a single group of animals to a large dose (the limit dose) of the test substance. A test substance that shows little or no effects at the limit dose is considered essentially nontoxic, and no further testing is needed. If compound-related mortality is observed at the limit dose, then further testing may be necessary.

4.3.2.2 Summary of Available Data

Acute toxicity data for the arylpolyolefin category is summarized in Table 7. Both category members have been tested for acute oral and acute dermal toxicity. A low order of toxicity was observed for both category members.

4.3.2.2.1 Acute Oral Toxicity

Both of the substances in the arylpolyolefin category have been adequately tested for acute oral toxicity in rats. For both of the substances in the arylpolyolefin category, no mortality was observed for the test material when administered at the limit dose of 5 g/kg. The acute oral LD_{50}s for these substances were greater than the 5 g/kg limit dose, indicating a relatively low order of toxicity.

4.3.2.2.2 Acute Dermal Toxicity

Both of the substances in the arylpolyolefin category have been adequately tested for acute dermal toxicity. For both of the substances in the arylpolyolefin category, no mortality was observed for the test material when administered to rabbits at the limit dose of 2 g/kg. The acute dermal LD_{50}s for these substances were greater than the 2 g/kg limit dose, indicating a relatively low order of toxicity.

4.3.2.3 Data Assessment and Test Plan for Acute Mammalian Toxicity

In total, four adequate acute toxicity studies have been conducted for the arylpolyolefin category members. These studies involved two species of laboratory animals (rats and rabbits); two routes of exposure (oral and dermal); and evaluated the toxicity of both members of the arylpolyolefin category. The data consistently demonstrate a low order of acute toxicity. The low order of toxicity observed for each of the substances in this group is consistent with their similar chemical structure. Therefore, the toxicity of the arylpolyolefin category has been evaluated adequately with respect to acute toxicity endpoints, and no additional acute toxicity testing is proposed.

4.3.3 Genotoxicity of the Arylpolyolefin Category

4.3.3.1 Genotoxicity Test Methodology

Genetic toxicology is concerned with the effects of substances on genetic material (i.e., DNA and chromosomes). Within genetic material, the gene is the simplest functional unit composed of DNA. Mutations are generally non-lethal, heritable changes to genes that may arise spontaneously or as a consequence of xenobiotic exposure. The propensity of a chemical to cause genetic mutations is commonly measured in bacterial and mammalian cells. The simplest test systems measure the occurrence of a base-pair substitution mutation in which a single nucleotide is changed followed by a subsequent change in the complementary nucleotide on the other DNA strand. Frame shift mutations occur following the deletion or insertion of one or more nucleotides, which then changes the "reading frame" for the remainder of the gene or multiple genes. Genetic testing for these types of point mutations is generally accomplished by *in vitro* cellular assays for forward or reverse mutations. A forward mutation occurs when there is a detectable change in native DNA whereas a reverse mutation occurs when a mutated cell is returned to its initial phenotype. Both base-pair substitutions and frame shift mutations are routinely measured in bacterial cells by measuring the ability of a cell to acquire the capability to grow in an environment missing an essential amino acid. In these tests, a large number of cells are examined to demonstrate a significant increase in the frequencies of mutations that occur over the frequency of spontaneous mutations.

Chromosomal aberrations are large-scale numerical or structural alterations in eukaryotic chromosomes including deletions (visualized as breaks), translocations (exchanges), non-disjunction (aneuploidy) and mitotic recombination. Chromosomal breakage is the classical end point in chromosomal aberration assays. Substances that induce structural changes in chromosomes, especially chromosome breaks, are referred to as "clastogens." To visualize chromosomes and chromosomal aberrations following *in vitro* or *in vivo* treatment with a substance, cells are arrested in metaphase, treated to swell the chromosomes, fixed, transferred to slides and stained. The first metaphase following treatment is the time at which the greatest number of cells with damaged chromosomes may be observed. The most frequently used test systems investigate changes in mammalian cells (such as Chinese hamster ovary or lung cells; human or rat lymphocytes; or human, rat or mouse bone marrow cells) following either *in vitro* or *in vivo* exposure to the test substance. The micronucleus test is a common *in vivo* assay that measures the frequency of micronuclei formation (i.e., chromosomal fragments) in polychromatic erythrocytes.

4.3.3.2 Summary of Genotoxicity Data

A summary of the genotoxicity information for the arylpolyolefin category is presented in Table 8. An *in vitro* bacterial gene mutation assays has been conducted for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9). No chromosomal aberration assays are available for the members of the arylpolyolefin category.

4.3.3.2.1 Bacterial Gene Mutation Assays

The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) has been tested using an *in vitro* bacterial gene mutation assay. The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) did not demonstrate mutagenic activity in the presence or absence of metabolic activation. This test will be used for bridging to the polypropene derivative (CAS # 68081-77-6).

4.3.3.2.2 Chromosomal Aberrations Assays

There are no chromosomal aberration assays available for the members of the arylpolyolefin category.

4.3.3.3 Data Assessment and Test Plan for Genotoxicity

No additional bacterial gene mutation assays are proposed for the arylpolyolefin category. The *in vitro* bacterial gene mutation data for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) will be bridged to the polypropene derivative (CAS # 68081-77-6). The C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) will be tested in an *in vitro* chromosomal aberration assay and the data will be bridged to the polypropene derivative (CAS # 68081-77-6).

4.3.4 Repeated-Dose Toxicity of the Arylpolyolefin Category

4.3.4.1 Repeated-Dose Toxicity Test Methodology

Repeated-dose toxicity studies evaluate the systemic effects of repeated exposure to a chemical over a significant period of the life span of an animal (rats, rabbits, or mice). Chronic repeated-dose toxicity studies are concerned with potential adverse effects upon exposure over the greater part of an organism's life span (e.g., one to two years in rodents). Subchronic repeated-dose studies are also concerned with effects caused by exposure for an extended period, but not one that constitutes a significant portion of the expected life span. Subchronic studies are useful in identifying target organ(s), and they can be used in selecting dose levels for longer-term studies. Typically, the exposure regimen in a subchronic study involves daily exposure (at least 5 consecutive days per week) for a period of at least 28 days or up to 90 days (i.e., 4 to 13 weeks). A recovery period of two to four weeks (generally included in most study designs) following completion of the exposure period provides information on whether or not the effects observed are reversible upon cessation of treatment. The dose levels evaluated in repeated-dose toxicity studies are notably lower than the relatively high limit doses used in acute toxicity studies. The NOAEL (no observed adverse effect level), usually expressed in mg/kg/day, is defined as the dose of test material that produces no significant toxicological effects. In some instances, the test material produces toxicity even at the lowest dose tested (i.e., there is no defined NOAEL); in these cases, the lowest dose that produced an adverse effect is defined as the LOAEL (lowest observed adverse effect level). Alternatively, results may be reported as the NOEL (no observed effect level) or the LOEL (lowest observed effect level) which are defined, respectively, as the highest dose of the test material that produced no treatment-related effects and the lowest dose that produced treatment-related effects. While these studies are designed to assess systemic toxicity, the study protocol can be modified to incorporate evaluation of potential reproductive and/or developmental effects.

Reproductive and developmental toxicity studies generate information on the effects of a test substance on male and female reproductive performance such as gonadal function, mating behavior, conception, development of the conceptus, parturition and post-partum development of the offspring. Various study designs exist, but they all involve exposure of both male and female animals to the test substance before mating. The rat is most often selected as the test species. The test substance is administered to males and females continuously at several graduated doses for at least two weeks prior to mating and until the animals are sacrificed. The males are treated for at least two more weeks. Male gonadal histopathology is assessed at the end of the study. The females are treated through parturition and early lactation. The adult females and offspring are typically studied until termination on post-natal day 21, or sometimes earlier. In addition to providing data on fertility and reproduction, this study design provides information on potential developmental toxicity following prenatal and limited post-natal exposure to the test substance. A NOAEL or LOAEL is also used to describe the results of these tests, with the exception that these values are derived from effects specific to reproduction or development.

4.3.4.2 Summary of Available Data

There are no repeated-dose or reproductive/developmental toxicity studies available for the members of the arylpolyolefin category.

4.3.4.3 Data Assessment and Test Plan for Repeated-Dose Toxicity

4.3.4.3.1 Repeated-Dose Toxicity

There are no repeated-dose toxicity studies available for the members of the arylpolyolefin category. An oral repeated-dose toxicity study will be conducted on the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the data will be bridged to the polypropene derivative (CAS # 68081-77-6).

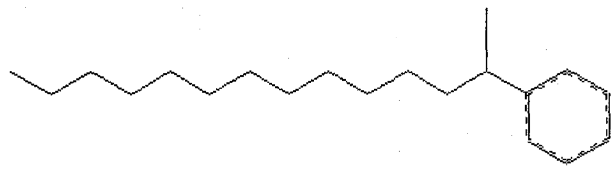
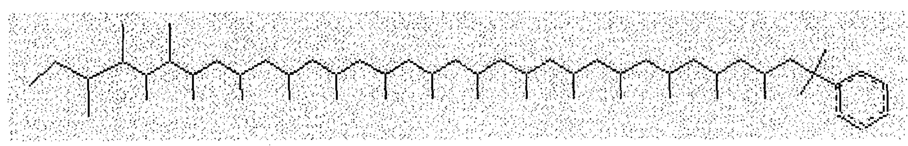
4.3.4.3.2 Reproductive/Developmental Toxicity

There are no reproductive or developmental toxicity studies available for the members of the arylpolyolefin category. A reproductive/developmental toxicity study will be conducted on the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and the data will be bridged to the polypropene derivative (CAS # 68081-77-6).

Table 1. Registration Numbers and Chemical Names for Arylpolyolefin Category Members

CAS Number	EINECS Number	Chemical Name	Simplified Chemical Name
115733-08-9	None	Benzene, C_{14}-C_{24}-branched and linear alkyl derivatives	C_{14}-C_{24} alkaryl derivative
68081-77-6	None	Benzene, polypropene derivatives	Polypropene derivative

Table 2. Chemical Structures and Names of Arylpolyolefin Category Members

CAS Number	Idealized Chemical Structure and Name
115733-08-9	 C_{14}-C_{24} alkaryl derivative [a]
68081-77-6	 Polypropene derivative [b]

[a] Structure represents the benzene C_{14} alkyl derivative.
[b] Structure represents an intermediate molecular weight range benzene polypropene (C_{52}) derivative.

Table 3. Selected Physicochemical Properties of Arylpolyolefin Category Members and Proposed Testing

CAS Number	Molecular Weight Range[1]	Specific Gravity (@ 15.6°C)	Viscosity (cSt @ 40°C)	Melting Range (°C)	Boiling Range[2] (°C)	Vapor Pressure Range[2] (Pa @ 25°C)	Water Solubility Range[2] (mg/L @ 25°C)	Log Kow Range[2]
115733-08-9	275-415	0.85	21	N.A.	342-458	$1.3e^{-2}$- $1.7e^{-6}$	$2.0e^{-4}$ - $4.4e^{-9}$ **Test**	8.9 - 13.8
68081-77-6	387-1228	0.87	93	N.A.	≥388	≤$6.2e^{-4}$	≤1.2^{-7}	≥12.3

[1] Based on molecular weight range of component molecules.
[2] Modeled data based on molecular weight range.
N.A. - Not applicable for liquids at ambient temperatures.

Table 4. Biodegradation, Hydrolysis and Photodegradation Data for Arylpolyolefin Category Members and Proposed Testing

CAS Number	BIODEGRADABILITY Available Data & Proposed Testing	HYDROLYSIS[1] Available Data & Proposed Testing	PHOTODEGRADATION[2] Available Data & Proposed Modeling
115733-08-9	**Test**	No testing proposed Arylpolyolefins are not subject to hydrolytic reactions	Direct Photodegradation: No testing needed - Arylpolyolefins are not subject to photolytic reactions Indirect Photodegradation: No testing needed Calculated OH^- Rate Constant (cm^3/molec-sec) = 23e-12 to 37e-12 Calculated Half-life in Air (hrs) = 5.67 to 3.49
68081-77-6	No testing proposed – Bridging	No testing proposed Arylpolyolefins are not subject to hydrolytic reactions	Direct Photodegradation: No testing needed - Arylpolyolefins are not subject to photolytic reactions Indirect Photodegradation: No testing needed Calculated OH^- Rate Constant (cm^3/molec-sec) = ≥31e-12 Calculated Half-life in Air (hrs) = ≤4.10

[1] Chemical components of arylpolyolefin products do not contain functional groups that are subject to hydrolytic reactions; these substances are expected to be stable in water and no testing is necessary.

[2] Chemical components of arylpolyolefin products do not absorb sufficient light energy to result in a structural transformation, therefore these substances are expected to be stable in solution and no testing is necessary; AOPWIN, a subroutine in EPIWIN, was used to model potential indirect photodegradation rates for selected chemical structures that represent arylpolyolefin category members (see Section 4.1.4.1).

Table 5. Distribution and Fugacity Data for Selected Chemical Components of Arylpolyolefin Category Members

CAS Number	PERCENT DISTRIBUTION AND FUGACITY[1]						
	Available Modeling Data						
	Air (%)	Water (%)	Soil (%)	Sediment (%)	Suspended Sediment (%)	Biota (%)	Fugacity (uPa)
115733-08-9 Benzene C_{14} alkyl derivative[a]	0.102	1.3e-4	97.7	2.170	0.068	0.005	9.18e-3
115733-08-9 Benzene C_{24} alkyl derivative[a]	0.026	1.8e-9	97.7	2.172	0.068	0.006	1.54e-3
68081-77-6 Benzene C_{22} polypropene[a]	0.027	5.5e-8	97.7	2.172	0.068	0.006	1.71e-3

[1] The EQC Level I model as referenced in Mackay et al., 1996 (Environ. Toxicol. Chem. 15:1627-1637), was used to calculate environmental partitioning data for selected chemical structures that represent arylpolyolefins (see Section 4.1.5.1).
[a] The structure used for modeling.

Table 6. Aquatic Toxicity Data for Arylpolyolefin Category Members and Proposed Testing

CAS Number	FISH ACUTE TOXICITY 96-hr LC_{50} (mg/L)	INVERTEBRATE ACUTE TOXICITY 48-hr EC_{50} (mg/L)	ALGA TOXICITY 96-hr EC_{50} (mg/L)
	Available Data & Proposed Testing	**Available Data & Proposed Testing**	**Available Data & Proposed Testing**
115733-08-9	**Test**	**Test**	**Test**
68081-77-6	No testing proposed – Bridging	No testing proposed – Bridging	No testing proposed – Bridging

Table 7. Evaluation of Acute Mammalian Toxicity of Arylpolyolefin Category Members

CAS Number	ACUTE ORAL TOXICITY[1]	ACUTE DERMAL TOXICITY[1]
	Available Data	Available Data
115733-08-9	$LD_{50} > 5$ g/kg (rat)	$LD_{50} > 2$ g/kg (rabbit)
68081-77-6	$LD_{50} > 5$ g/kg (rat)	$LD_{50} > 2$ g/kg (rabbit)

[1] Toxicity endpoints are expressed as median lethal dose (LD_{50}) for acute oral and dermal toxicity. The LD_{50} is defined as the dose that is lethal to 50% of the test organisms. The greater the LD_{50}, the lower the toxicity.

Table 8. Evaluation of Genotoxicity of Arylpolyolefin Category Members and Proposed Testing

CAS Number	GENE MUTATION ASSAY	CHROMOSOMAL ABERRATION ASSAY
	Available Data & Proposed Testing	**Available Data & Proposed Testing**
115733-08-9	*In vitro* Bacterial Reverse Mutation Assay – With and Without S-9 – Not Mutagenic	**Test**
68081-77-6	No testing proposed – Bridging	No testing proposed– Bridging

Table 9. Evaluation of Repeated-Dose Mammalian Toxicity of Arylpolyolefin Category Members and Proposed Testing

CAS Number	REPEATED-DOSE TOXICITY	REPRODUCTIVE/DEVELOPMENTAL TOXICITY
	Available Data & Proposed Testing	Available Data & Proposed Testing
115733-08-9	**Test**	**Test**
68081-77-6	No testing proposed – Bridging	No testing proposed – Bridging

Table 10. Summary of Data for Arylpolyolefin Category Members and Proposed Testing

CAS Number	Environmental Fate					Ecotoxicity			Human Health Effects				
	Physical Chem	Photodeg	Hydrolysis	Fugacity	Biodeg	Acute Fish Toxicity	Acute Invert Toxicity	Algal Toxicity	Acute Toxicity	Point Mutations	Chrom Effects	Sub-chronic	Repro/ Develop
115733-08-9	C / T	D / C	D	C	T	T	T	T	A	A	T	T	T
68081-77-6	C / B	D / C	D	C	B	B	B	B	A	B	B	B	B

A Adequate data available
B Bridging
C Computer modeling completed
D Technical discussion completed
T Test